beta-Ocimene

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.95	0.69	0.95	0.65	0.96	0.68

Model Results

Predicted value: 4.47

Global applicability domain: Inside

Local applicability domain index: 9.79e-01

Confidence level: 6.40e-01

Nearest Neighbors from the Training Set

Image not found	Image not found	Image not found
1,2-Dichlorobenzene	Propylbenzene	1,3-Dichlorobenzene
Measured: 4.36	**Measured:** 4.09	**Measured:** 4.12
Predicted: 4.46	**Predicted:** 4.53	**Predicted:** 4.44

Image not found	Image not found
Octanal	1,4-Dichlorobenzene
Measured: 5.36	**Measured:** 4.46
Predicted: 4.54	**Predicted:** 4.45